

The importance of the spectral gap in estimating ground-state energies

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We study the role played by the spectral gap in the complexity of the LocalHamiltonian problem. To do so, we consider the setting in which one estimates the ground-state energy to within inverse exponential precision. In this setting, the complexity of LocalHamiltonian is magnified from QMA to PSPACE. We show that the full complexity of the high precision case only comes about when the spectral gap is exponentially small. We also obtain implications for the representability and circuit complexity of ground states of local Hamiltonians, uniqueness of quantum witnesses, and amplification of quantum witnesses in the presence of postselection.

Keywords: Complexity theory, spectral gap, PSPACE, PP

Finding effective descriptions of ground states of many-body Hamiltonians on n qubits is a very natural and important task in physics. Given the prevalence and importance of this task, an important question is that of the computational difficulty of solving this task in naturally occurring situations, which can be formalized through the LOCALHAMILTONIAN problem [1, 2]. One quantity that plays a huge role in the ground-state physics of a Hamiltonian is the spectral gap, whose role in the context of the LOCALHAMILTONIAN problem is much less clear. In particular, it is not known whether LOCALHAMILTONIAN is QMA-complete in the presence of nontrivial lower bounds on the spectral gap [3–6].

In this work [7], we take an initial step towards understanding the role played by the spectral gap in the LOCALHAMILTONIAN problem. To do so, we study QMA in the precise setting, i.e. the class PreciseQMA, which translates to computing the ground-state energy to within inverse-exponential precision in the system size. Fefferman and Lin [8] studied the complexity of this class and showed the mysterious result that it equals PSPACE. This is surprising since $\text{QMA} \subseteq \text{PP}$ [9–11], and an alternative characterization of the class PP is PreciseBQP, which can handle inverse-exponentially small promise gaps.

We provide an explanation for the unexpected boost in complexity from QMA to PSPACE. Specifically, we find that in order for the precise version of LOCALHAMILTONIAN to be PSPACE-hard, the spectral gap of the Hamiltonian must necessarily shrink superpolynomially with n . We give strong evidence that if the spectral gap shrinks no faster than a polynomial in the system size, the complexity of the problem is strictly less powerful. In particular, we show that this problem characterizes the complexity class PP, which is a subset of PSPACE and is widely believed to be distinct from PSPACE. Our results therefore bring out the importance of the spectral gap, a quantity not well un-

derstood so far in Hamiltonian complexity.

Another main result of ours concerns the existence of polynomial-size quantum circuits to prepare ground states of local Hamiltonians. This is an important question that has implications in circuit-complexity of ground states of natural Hamiltonians and is directly related to whether natural Hamiltonians can be efficiently cooled down to zero temperature. In complexity-theoretic language, this is phrased in terms of the power of classical versus quantum witnesses in Merlin-Arthur proof systems, or more formally, the so-called QMA vs. QCMA question. These classes are believed to be inequivalent in the usual [12, 13] and precise [14, 15] regimes. Interestingly, we show strong *equivalence* results for the PreciseQMA vs. PreciseQCMA question in the presence of spectral gaps.

Our results are summarized in the table below and mention the complexity of computing the ground-state energy of a Δ -gapped Hamiltonian to precision δ . For the second and third columns, there is a promise that there is a circuit (a classical witness) to prepare a low-energy state, while the last two columns have no such promise.

Spectral gap (Δ)	Classical witness		Quantum witness	
	$\delta = 1/\text{poly}$	$\delta = 1/\text{exp}$	$\delta = 1/\text{poly}$	$\delta = 1/\text{exp}$
1/poly	QCMA	PP	PGQMA [3]	PP
1/exp	QCMA	NP ^{PP}	?	PSPACE
0	QCMA	NP ^{PP}	QMA [1]	PSPACE [8]

TABLE I: Complexity of variants of the LOCALHAMILTONIAN problem as a function of δ , the precision, and Δ , the spectral gap. The problem is complete for the class mentioned in each cell. The question mark indicates that the problem is uncharacterized. All results except the ones with a citation are from our work [7].

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